

Causes of Color in Minerals and Gemstones

Paul F. Hlava
Sandia National Laboratories
Department 1822
Mail Stop 0886
Albuquerque, NM 87185-0886

The colors that one sees when looking at a mineral or gemstone are due to the response of that person's eye to the energies of the light, the emission spectrum of the illumination, and, most importantly, physical phenomena in the material that cause some colors to be absorbed while others are undisturbed or enhanced. It is beyond the scope of this talk to do more than touch on the physiology of the eye that allows us to see colors. Likewise, we will not dwell on the emission spectra of various light sources. Rather, we will concentrate on the various ways in which materials, especially minerals and their heights of perfection - gemstones, produce color from white light.

Light is a form of energy (electromagnetic energy) and white light is a mixture of all of the visible energies (or wavelengths). In order for a mineral to cause color from white light it has to somehow perturb the balance of the light energies. Kurt Nassau^{2,3} has separated the causes of color into 15 mechanisms based on 5 physical groupings. While there are some color mechanisms that depend on direct emission of certain colors, most of the mechanisms we are interested in depend on the ability of minerals to preferentially absorb certain energies of light. When these energies are removed from the white light the mineral is colored by the complimentary color as demonstrated by the CIE* Chromaticity Diagram.

Light absorption by the electrons of transition metal (or rare earth element - REE) atoms, either as major portions of the mineral chemistry or impurities, is one of the most important and well known of the coloring mechanisms^{2,3,5}. Most common, rock-forming elements have electronic structures which mitigate against causing colors. On the other hand, transition metals (and REE's) have electrons which can be excited to open, higher energy levels. The electrons gain the necessary energy for the excitation by absorbing a particular energy (color) from white light and thus cause the mineral to show the complimentary color. Three prime examples of this mechanism are rubies, emeralds, and alexandrites but there are many, many more.

The second most important and common coloring mechanism is intervalence charge transfer. This occurs when a valence electron from one atom transfers to the structure of a close-by atom (often of a completely different element) again by absorbing just the amount of energy needed to make the transfer. Examples include sapphire, lapis lazuli, and amazonite.

Color centers (also known as F-centers or farbe {German for color} centers) are created when atoms are oxidized or removed. This is usually done by radiation. In most cases the hole left behind is occupied by an electron trying to proxy for the missing atom. This electron comes from a neighboring atom and the unpaired electron left behind is prone to absorb light energy and thereby create colors. The most familiar examples of minerals colored by color centers are amethyst and smoky quartz but fluorite, green diamonds, and brown topaz are also good examples. Color centers are one of the few coloring mechanisms that can be removed by heating or exposing the mineral to strong light.

Band gap colors are produced in insulating and semiconducting materials. They require an energy gap between the valence and conduction energy in the electronic structure of an atom. If the energy band includes all wavelengths of light the material is white or clear and an insulator. If the band includes the energies of part of the visible spectrum the material is a semiconductor and colored. Some insulators can be band-gap colored by impurities. Examples of minerals colored by band gap mechanisms are diamonds, cinnabar, and cuprite.

Scattering of light can cause colors to appear because blue light is more prone to scattering than red. Scattering is caused by submicroscopic (the finer the better) grains of solid or liquid, material. It can even be caused by random collisions of gas molecules in the atmosphere. Scattering is responsible for the blue of the sky, the white of clouds (and bull quartz), and the red color of sunsets. Minerals that display a special case of scattering are moonstones, cat's eyes, and asterated (star) stones.

Interference colors are caused when light travels obliquely through materials with thin layers of differing refractive index. The layers have to be about as thick as a wavelength of light. A coherent ray of light shining through the material is dispersed in the new medium. At each interface some of the light is reflected back up and some continues on down. If the layers are of such a thickness that a particular color is retarded by exactly one or a few integral wavelengths, the reflected ray of color and its refracted then reflected counterpart will constructively interfere with each other and that color will be bright. Those colors that are an integer and one half retarded will be destructively interfered and therefore cancelled out. Retardations between those extremes are muted. The effect is the schiller we associate with oil slicks, labradorite, cryptoperthite-type moonstones, etc.

Diffraction can be considered a special case of interference caused, not by lamellae, but by layers of fine spheres. Each sphere scatters the light impinging on it in a radial fashion. As the layers are tilted, different wavelengths are constructively interfered with in different directions producing not one color but a play of colors. The spheres have to be perfectly round, of the same, exact size (about the size of light waves), and packed into perfect order or the play of colors will be killed. The perfect example is precious opal. An imperfect example is the rainbow of colors one see when viewing a bright source of light through a fine screen or the cloth of an umbrella.

*Commission Internationale de l'Eclairage

Acknowledgements, References, and Suggested Reading

1. This work was supported by the United States Department of Energy under Contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.
2. Kurt Nassau, "The Physics and Chemistry of Color: The Fifteen Causes of Color", John Wiley & Sons, New York, 1983, 454 pp.
3. Kurt Nassau, "The Causes of Color", Scientific American, vol. 243, no. 4, Oct., 1980, pp. 124 - 154 (Provides an excellent summary of the subject.)
4. Kurt Nassau, "Cubic Zirconia: An Update", Gems and Gemology, vol 17, no. 1, Spring 1981, pp. 9 - 19
5. Emmanuel Fritsch and George R. Rossman, "An Update on Color in Gems, Part 1: Introduction and Colors Caused by Dispersed Metal Ions", Gems and Gemology, vol 23, no. 3, Fall 1987, pp. 126 - 139
6. Kurt Nassau and G. Kay Valente, "The Seven Types of Yellow Sapphire and Their Stability to Light", Gems and Gemology, vol 23, no. 4, Winter 1987, pp. 222 - 231
7. Emmanuel Fritsch and George R. Rossman, "An Update on Color in Gems, Part 2: Colors Involving Multiple Atoms and Color Centers", Gems and Gemology, vol. 24, no. 1, Spring 1988, pp. 3 - 15
8. Emmanuel Fritsch and George R. Rossman, "An Update on Color in Gems, Part 3: Colors Caused by Band Gaps and Physical Phenomena", Gems and Gemology, vol 24, no. 2, Summer 1988, pp. 81 - 102 -- (Contains a table describing the causes of color for most gemstones.)
9. Emmanuel Fritsch et al., "Gem-Quality Cuprian-Elbaite Tourmalines from São José da Batalha, Paraíba, Brazil", Gems and Gemology, vol 26, no. 3, Fall 1990, pp. 189 - 205

“Gems and Gemology” contains numerous articles that include discussions of particular coloring mechanisms (such as ref. 9). Too many to be enumerated here.



Fig. 1 These two photos illustrate 3 examples of coloring mechanisms. The star sapphire is colored by intervalence charge transfer while the star is caused by scattering. The Hope diamond illustrates band gap color.